REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
		FINAL REPORT - 15 Nov 94 - 14 Nov 96

4. TITLE AND SUBTITLE
Ultraviolet Emission Cross Sections by Electron Impact: Application to UV Dayglow and Auroral Satellite Observations

5. FUNDING NUMBERS
61102F
2301/DS

6. AUTHOR(S)
Professor Ajello

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Laboratory for Atmospheric and Space Physics
University of Colorado
Boulder, CO 80302

AFOSR-TR-97
0174

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NE
110 Duncan Avenue Suite B115
Bolling AFB DC 20332-8050

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
F49620-95-1-0069

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

This program has developed for the Air Force a high resolution spectrometer, including EUV and FUV array detectors, which is the highest resolution single-scattering instrument available in the US for the measurement of emission cross sections. Electron impact induced fluorescence studies have been made of emission spectra of atomic hydrogen and of molecular hydrogen, nitrogen, and oxygen,. Three fully operational UV emission cross section instruments, ranging in resolving power from low resolution for the atomic studies to high resolution for molecular studies, were used. For each species, a model was developed that included collision strengths in analytic form for routine addition to energy loss codes or spectral models which are then applied to model radiative/collisional equilibrium in the earth's thermosphere. Air Force satellite and rocket programs use atomic and molecular cross sections from this program in the development of atmospheric models for the data analysis phase of missions. Examples of these flight programs are the recent analyses of the Air Force UV GLOW experiment (Strickland, 1996) and the Phillips Laboratory rocket-borne spectrometer (Eastes and Dentamaro 1996; Eastes and Sharpe, 1987).

14.

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	

FINAL TECHNICAL REPORT

TITLE: ULTRAVIOLET EMISSION CROSS SECTIONS BY ELECTRON IMPACT: APPLICATION TO UV DAYGLOW AND AURORAL SATELLITE OBSERVATIONS

AGENCY: Air Force Office of Scientific Research

Grant Number: F49620-95-1- 0069

Principal Investigator: Joseph Ajello
Laboratory for Atmospheric and Space Physics
Univesity of Colorado
Boulder, CO 80302

Program Manager: Dr. Ralph E. Kelley

1.0 INTRODUCTION

The development of the high resolution spectrometer including EUV and FUV array detectors represents the highest resolution single-scattering instrument available in the US for the measurement of emission cross sections.is the major result of this laboratory program for the Air Force. In the laboratory program, we use electron impact induced fluorescence studies of Terrestrial gases as the primary method of investigation. The To acquire the data base there are three fully operational UV emission cross section instruments, ranging in resolving power from low resolution ($\lambda/\Delta\lambda$=1000) for the atomic studies to high resolution ($\lambda/\Delta\lambda$=67000) for molecular studies under the control of a staff of 5 Ph.D. scientists, composing the UV Emission Processes Group (http: //schroedinger.jpl.nasa.gov). For each species studied, we develop a model atom with collision strengths. The collision strengths are put in analytic form for routine addition to energy loss codes or spectral models which are then applied to radiative/collisional equilibrium in the Earth's Thermosphere.

Air Force, Navy, DOD and NASA satlellite and rocket programs make use of the atomic and molecular cross sections from this program in the development of atmospheric models for the data analysis phase of its missions. Examples of these flight programs since 1990 were the recent analysis of Air Force UV GLOW experiment (Strickland, 1996, private communication), Phillips Laboratory rocket-borne spectrometer (Eastes and Dentamaro 1996; Eastes and Sharpe, 1987), Berkeley's EUV rocket-borne spectrometer (Cotton et al., 1993) and Navy Ultraviolet Limb (UVLIM) observations of the dayglow and aurora from the Space Shuttle (Budzien et al., 1994)).

The Earth-orbiting satellites (Dynamics Explorer, Polar Bear, Shuttle GLOW , MSX , Atlas, and Polar, RAIDS), (Torr et al., 1994, 1995, Meier et al,, 1995, Budzien et al., 1995) and sounding rockets (Cotton et al., 1995, Morrison et al., 1990, Link et al., 1988), have established that band systems of N_2 and the atomic emissions of O are the dominant emissions in the terrestrial UV airglow and aurora produced by electron impact. The CU/JPL model is currently used as the basis for energy loss codes describing electron energy degradation in the Earth's atmosphere by the Air Force (Strickland et al., 1989; Link et al., 1988, Huffman et al., 1989). A recent compilation of aeronomical cross sections for N_2 , O_2 , O used in the modeling codes for evaluation of Air Force observations by Dr. D. Strickland and T. Majeed (Majeed et al., 1996) shows a general use of CU/JPL cross sections developed in this program eg. N_2(a,b,b',c_4',C) (Ajello et al., 1985,1989; James et al., 1990; .Shemansky et al., 1995a,b).

1.1 RESEARCH OBJECTIVES:

1. Laboratory studies to remeasure the N_2 (a $^1\Pi_g$) state cross section and estimate contributions from radiative and collisional cascade from the metastable a' and w-states, the a $^1\Pi_g$ state, the upper state of the LBH bands, is the most important cross section for the AF observations of the UV airglow of the Earth in the next decade.

2. Measure cross sections of HI Lyman series and OI(98.9, 102.5, 130.4, 135.6 nm) emissions with two instruments dedicated to study the radical species H and O in the UV. Atomic oxygen emissions account for 90% of the FUV airglow/aurora and over 50% of EUV airglow/aurora.

3. Laboratory studies will measure predissociation yields, experimental Franck-Condon factors, band oscillator strengths (f), collision strengths, and UV emission cross sections over the energy range 0-2 keV for Rydberg and valence electronic states (5-15 eV) of the diatomic molecules: H_2, N_2, HD, D_2, CO, NO, O_2. The purpose is to provide atomic parameters and cross sections for modeling and planning UV observations from Earth satellites (SMX, DMSP, Polar, RAIDS, HUT, Shuttle GLOW, Atlas) and interplanetary spacecraft (Voyager, Galileo, CRAF-CASSINI). Emphasis will be given to N_2 (b,b',c_4') and H_2 (B,B',B'',C,D,D') states. *Ab initio* theories of configuration interaction, require accurate band intensities, experimental Franck-Condon factors, wavelengths and branching ratios. Collaborations with the Meudon Observatory allow us access to the latest published theoretical data files of transition probabilities and wavelength.

4. Detailed electron low energy (0-50 eV) studies at low (0.1-1 nm) and medium spectral resolution (0.01-1nm) of resonance effects, threshold

cross sections and optically forbidden excitation of H_2, N_2, O_2, NO. This is an important energy range where secondary electron distributions tend to peak in the aurora, dayglow, and electroglow of the Earth and other planetary atmospheres. *Ab initio* calculations require accurate experimental benchmark data to test low energy theories.

5. Standard low and medium resolution electron impact induced fluorescence spectra and array detector band imaging and spectroscopic models at 100 and 200 eV of N_2, H_2, O_2, NO, CO available on SPAN and INTERNET. These spectra will serve to calibrate space instrumentation and for testing simple spectral models to be used in analyzing spectra from the Earth's airglow and aurora. More complex models of configuration interaction require experimental measurements of rovibronic band intensities.

6. Measure Doppler line profiles of the fast atoms of N and O produced in the dissociative excitation of N_2, NO and O_2, including the resonance lines, N(120.0 nm) and O(130.4 nm).

2.0 UV EMISSION LABORATORY

The measurement of electron impact induced emission cross sections of stable atoms and molecules is currently performed in the UV Emission Laboratory. The Laboratory consists of three independent UV spectrometer systems each with an electron beam-molecular beam collision chamber in tandem with a UV spectrometer, interfaced with a computer for automatic data acquisition. These systems are capable of: 1) high spectral resolution, resolving power $\lambda/\Delta\lambda$ = 67,000, for studying rotational structure and kinetic energy of excited fragments, 2) medium spectral resolution, resolving power $\lambda/\Delta\lambda$ = 5000, for studying continuous and discrete absorption processes (currently being used to study N_2 and O_2 in the FUV, and 3) two low spectral resolution instruments, resolving power $\lambda/\Delta\lambda$ = 1000 for studying whole band systems of stable gases and equipped with an atomic beam sources for generation of atomic radicals by RF and microwave techniques for H and O, respectively. Each UV spectrometer has dual exit ports to allow scanning over two wavelength ranges, for example the EUV (40-120 nm) and FUV (110-310 nm), without breaking vacuum. The high resolution spectrometer is custom designed and is equipped with four exit and two entrance ports. All of the instruments are operational and producing state-of-the-art data except for the atomic oxygen apparatus which is the final design and construction stage (described below).

For each species studied, UV emission spectra are measured by crossing a collimated beam of electrons with a beam of target gas formed by a capillary array at a background pressure that ensures optically thin conditions. Emitted

photons, corresponding to the radiative decay of collisionally excited states of the target species, are detected by the UV spectrometer. The calibration paper published in Applied Optics (Ajello et al., 1988; Liu et al., 1995) discusses the JPL EUV and FUV laboratory calibration techniques. These techniques coupled with the relative flow calibration also developed at JPL(Kanik, 1996)), allows a determination of absolute cross sections from an optical system.

Excitation function measurements, performed in the swarm mode by ramping the electron beam energy within the range 0-2 keV, can be put on an absolute scale by normalization to the UV spectra measured at discrete impact energies. These energy scans extend well into the region where the Born approximation is valid for the determination of optical oscillator strengths.

2.1 ATOMIC OXYGEN EXPERIMENTAL APPARATUS

The goal of the atomic oxygen laboratory program is to measure accurate emission cross sections of OI(1304 and 1356 Å) in the UV. As part of this goal it is important to simultaneously measure in the visible/near IR the OI emissions that provide cascade contributions. The design of the atomic oxygen apparatus is based on our five year program to study the $e + H \rightarrow H L_\alpha$ benchmark cross section to 10% accuracy (James et al., 1997). In the course of the atomic hydrogen program we have developed intense atomic beams and accurate calibration techniques - two problems that plagued earlier work on atomic H radicals. For the study of atomic O, recent experiments have been able to achieve high beam densities by microwave techniques (Wang and McConkey, 1992; Gulcicek and Doering, 1988). However, the two sets of absolute cross sections (Wang and McConkey; Zipf and Erdman, 1985) for the principal resonance line OI (1304 Å) cross section differ by 100% in the important low energy range of 15-25 eV. This is the energy regime in the daylglow and aurora where secondary electron distributions make a large contribution to the excitation process. After careful review of the Stone and Zipf (1974) experiment to measure the emission cross section of the forbidden OI(1356 Å) transition, the remeasurement of the absolute cross section can be best achieved by a combination energy-loss and emission techniques. The emission technique of this proposal provides the relative cross section as a function of energy. The energy-loss technique gives the direct excitation cross section (Doering and Gulcicek., 1989) and the emission experiment of this proposal in the visible supplies the cascade cross section at 20 eV. The sum of the two cross sections provides the reference cross section for the OI(1356 Å) excitation function, provided by this program.

The atomic oxygen apparatus is in the final construction stage. It consists of two apparatus in a single collision chamber capable of performing the following measurements : 1) UV emission cross sections (400-1400 Å) of the atomic radiation from the highly excited states of atoms which radiate to the ground state ($ns\ ^{3,5}S \rightarrow\ ^3P$; 989, 1025, 1152, 1216, 1304 and 1356 Å - the latter two are the targets of the NSF program), and 2) Visible/near IR emission cross section of cascade transitions to the $ns\ ^{3,5}S$ states by the $np\ ^{3,5}P$ Rydberg series

(8436 and 7774 Å, the first members of each Rydberg series, respectively, make the largest cascade contribution). A third mode is available for future studies of long lived metastables-time-of-flight (TOF) measurements of metastable atoms. A channeltron is located directly below the gas jet on a rail to detect the $^5S_2$ or other metastable states of atomic oxygen by a TOF technique as a function of distance from the beam source.

3.0 RESEARCH RESULTS :

In the last funding period of April 1994 to present the CU/JPL team has published twenty papers. The highlights of the program related to this study are the following:

3.1 MOLECULAR HYDROGEN: Published as: X. Liu et al. "High-Resolution Electron Impact Study of the Far Ultraviolet Spectrum of Molcular Hydrogen", Ap. J. Supp.110, 375 (1995).

The emission spectrum of molecular hydrogen produced by electron-impact excitation at 100 eV has been measured in the wavelength range 1140-1690Å. High-resolution, optically thin spectra ($\Delta\lambda$ = 0.136Å) of the far-ultraviolet (FUV) Lyman and Werner band systems have been obtained with a 3m spectrometer. Synthetic spectral intensities based on the transition probabilities calculated by Abgrall et al. are in very good agreement with experimentally observed intensities.

3.2 ATOMIC HYDROGEN: Published as: G. James et al., "The Electron Excitation Function of H Lyman-α From Threshold To 1800 eV" ,Phys. Rev. A, 55, 1069 (1997)

The excitation function of prompt Lyα radiation, produced by electron impact excitation of atomic hydrogen in the energy range from threshold to 1800 eV, has been measured in a crossed-beam experiment. The measured excitation functions shows excellent agreement in shape with recent theoretical convergent close coupling (CCC) calculations over a two order of magnitude range in energy.

3.3 MOLECULAR HYDROGEN: Published as: J. Ajello et al., "Kinetic Energy Distribution of H(2p) atoms from Dissociative Excitation of H_2", Phys. Rev. Lett.,75, 3261 (1995).

The kinetic energy distribution of H(2p) atoms resulting from electron impact dissociation of H_2 has been measured by an ultraviolet (uv) spectroscopic technique. Slow H(2p) atoms with peak energy near 80 meV produce the peak profile, which is nearly independent of impact energy. The wings of H Lα arise from dissociative excitation of a series of doubly excited Q_1 and Q_2 states, which define the core orbitals.

3.4 MOLECULAR HYDROGEN: Published as: X. Liu et al., "Excitation Cross Sections of the Lyman and Werner Band System of Molecular Hydrogen, J. Geophys. Res. , (In Press ,1997).

The excitation functions of the Lyman and Werner band systems of molecular Hydrogen have been measured from 15 to 1200 eV by measuring individual roational line cross sections.

3.5 MOLECULAR HYDROGEN: Published as: J. Ajello et al., "Line Profile of H Lyman α from Dissociative Excitation of H_2", J. Geophys. Res., 100, 3261 (1995).

A high-resolution uv spectrometer was employed for the first measurement of the H Lα emission Doppler profile from dissociative excitation of H_2 by electron impact. Analysis of the deconvolved line profile reveals the existence of a narrow central peak of 40 ± 4 mÅ FWHM and a broad pedestal base about 240 mÅ wide.

3.6 MOLECULAR HYDROGEN: Published as: J. Ajello et al., "Line Profile of H Lyβ from Dissociative Excitation of H_2", Phys. Rev. A., 53, 2303 (1996).

A high-resolution ultraviolet (UV) spectrometer was employed for the first measurement of the H Lyb emission Doppler line profile at 1025.7 Å from dissociative excitation of H_2. Analysis of the deconvolved line profile reveals the existence of a narrow central peak, less than 30 mÅ full-width-half-maximum (FWHM) and a broad pedestal base about 260 mÅ FWHM. Using two different techniques, the absolute cross section of HLb is found to be $3.28 \pm 0.80 \times 10^{-19}$ cm^2 at 100 eV electron impact energy.

3.7 MOLECULAR DEUTERIUM : Published as: H. Abgrall et al. "High-Resolution Electron Impact Study of the Far Ultraviolet Spectrum of Molcular Deuterium", Ap. J. (In Press, 1997).

The emission spectrum of molecular hydrogen produced by electron-impact excitation at 100 eV has been measured and modeled in the wavelength range 114-169 nm.

3.8 MOLECULAR HYDROGEN: Published as: H. Abgrall et al."The Emission Continuum of electron excited molecular Hydrogen", Ap. J. (In Press, 1997).

The emission continua of molecular hydrogen produced by the dissociation transitions of $^1\Sigma_u^+$ nps (B, B', B'', n=2,3,4) and $^1\Pi_u$ npp (C, D, D', D'', n=2,3,4,5) $\rightarrow$ X $^1\Sigma_g^+$ Rydberg has been measured and calculated in the wavelength range 114-169 nm. Synthetic spectra are in excellent agreement with high resolution laboratory spectra at 100 eV.

3.9 MOLECULAR NITROGEN: Published as: D.Shemansky et al., "Fine-Structure Branching in N_2 c_4' $^1\Sigma_u^+$ (0)", Ap. J. 452, 480 (1995).

We report a quantitative measurement of the predissociation fraction in the N_2 $c'_4{}^1\Sigma^+_u$ - $X\,{}^1\Sigma^+_g$ (0,0) band, with an experimental determination of rotational line strengths. The fine structure of the N_2 (c'_4-X) (0,0) band has been analyzed in optically thin laboratory emission spectra obtained from crossed electron and N_2 beams. The distortion of the emission envelope from calculations based on constant rotational level radiative transition probabilities and a thermalized ground state source population has been used to obtain an estimated predissociation loss fraction of 0.15 for the N_2 c'_4 (0) level averaged over rotational structure at a neutral gas temperature of 300K. The analysis has been aided by measurements at gas temperatures depressed over a range from 300 to 30 K. The predissociation rate is temperature dependent, caused by nonuniform predissociation at intermediate and high rotational levels. The coupling of the rotational branches, also measured quantitatively for N_2 c'_4 (0) for the first time in this experiment is complicated by configuration mixing with the $c_3\,{}^1\Pi_u$ and $b\,{}^1\Pi_u$ states forcing strong departures from Hönl-London factors.

3.10 MOLECULAR NITROGEN: Published as: D.Shemansky et al., "Electron Excitation Functions of the N_2 Second Positive System", Ap. J. 452, 472 (1995).

The band strengths of the electron excited N_2 ($C\,{}^3\Pi_u$ - $B\,{}^3\Pi_g$) second positive system (2PG) have been measured in the middle ultraviolet (MUV) range (280 - 444 nm). The energy dependence of the (0,0) and (1,0) band cross sections is reported with analytic shape functions for use in model calculations. The excitation functions were measured at low pressure to avoid effects of collisional cascade from higher lying states. At low electron energies (11-15 eV), the resolution and energy spacing of the excitation function measurements were sufficient to reveal the importance of threshold effects from resonance processes. The absolute cross section of the 337.1 nm band has a peak value of $1.11 \pm 0.15 \times 10^{-17}$ cm^2 at 14.1 eV. Above 30 eV the cross section decreases with an asymptotic E^{-2} dependence. A spectral analysis of the 2PG band system at 14 eV and 20 eV has provided relative excited state vibrational level cross sections. The variation of the electronic transition moment over the wavelength range indicated above, has been derived, and an improved transition probability matrix has been obtained. The rate coefficient for solar photoelectron excitation off the (0,0) band is 9.12×10^{-10} $cm^3\,s^{-1}$ for photoelectrons above 11.0 eV, a factor of about 1.3 smaller than the previous recommended value.

3.11 MOLECULAR NITROGEN: Published as: J. Ajello et al.,"Fast Nitrogen Atoms from Dissociative Excitation of N_2 by Electron Impact", J. Geophys. Res. 101, 18,953 (1996).

The Doppler profiles of one of the fine structure lines of the NI(1200 Å) g $^4S^0$ --^4P multiplet and of the NII(1085 Å) g $^3P^0$--^3D multiplet have been measured. Excitation of the multiplets is produced by electron impact dissociative excitation of N_2. The full-width-half-maximum (FWHM) is measured by a high resolution UV spectrometer (l/Dl = 50000). The experimental line profiles are evaluated by fast Fourier transform (FFT) techniques and analysis of the profiles yields the kinetic energy distribution of fragments. The FWHM of NI(1200 Å) increases from 27 ± 6 mÅ at 30 eV to 37± 4 mÅ at 100 eV as the emission cross section of the dissociative ionization excitation process becomes more important relative to the dissociative excitation process. The kinetic energy distribution function of the two fragment NI atoms at 30 eV impact energy is much broader than thermal with a FWHM of 5 ± 1 eV. The FWHM of the NII(1085 Å) line is 36± 4 mÅ and is produced only by dissociative ionization excitation. At 100 eV impact energy the FWHM of each of the emission line profiles of the NI(1200 Å) and NII (1085 Å) atoms indicates that the kinetic energy distribution is described by 10 ± 2 eV FWHM. Dissociative excitation processes are shown to be a small part of the total quantum yield of NI atoms. However, all types of dissociation processes appear to produce NI atoms with kinetic energy distributions having mean energies above 0.5 eV and can lead to a substantial escape flux of NI atoms from the satellites, Titan and Triton of the outer planets.Line-width studies of the fine-structure lines are paramount for understanding the radiative transfer of the NI (1200 Å)multiplet in the Earth's thermosphere (Meier, 1991).

3.12 Earth: M. Torr et al., "A Far Ultraviolet Imager for the International Solar-Terrestrial Physics Mission", in The Global Geospace Mission edited by: C. T. Russell (Kluwer Academic Publishers: Boston, 1995), p.329.

Dr. J. Ajello is a co-investigator on the UVI instrument for the Polar mission. The data analysis tools utilize the electron impact cross sections measured in this program. The global scale phenomenon represented by the aurorae as viewed in the LBH bands of N_2 and atomic O(1304, 1356 Å) contains considerable information concerning the solar-terrestrial connection. acquired images of the Auroral oval and polar cap not only yield the temporal and spatial morphology from which we can infer activity indices, but in conjunction with simultaneous measurements made on spacecraft at other locations within the magnetosphere, allow us to map the various parts of the oval back to their source regions in the magnetosphere. This paper describes the Ultraviolet Imager for the Global Geospace Sciences portion of the International Solar-Terrestrial Physics program.

REFERENCES

Wang, S. and J. W. McConkey, J. Phys. B. 25, 5461 (1992).
Gulcicek, E. E. and J. P. Doering, J. Geophys. Res., 94, 1541 (1989).
Ajello, J. M., J. Chem. Phys., 55, 3156 (1971).
Doering, J. P. and E. E. Gulcicek, J. Geophys. Res. 94, 2733 (1989).
Noren, C. and J. W. McConkey ??????
Ajello, J. et al., Appl. Optics 27, 890 (1988).
Kanik, I, Chem. Phys. Lett., In Press (1996).
Long, R. L., D. M. Cox and S. J. Smith, Phys. Chem., 72A, 521 (1968).